# Configuration Space and Second Quantization[1]

by
Vladimir Aleksandrovich Fock (in Leningrad)

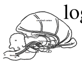
*December 22, 1898 – December 27, 1974*

Received March, 10th, 1932

(*Zeitschrift für Physik*, Vol. 75(9–10), page 622–647, 1932)

[1]The content of this work was presented in the theoretical seminar at the University of Leningrad in January 1931; However, due to external circumstances, the publication was delayed.


$$\oiiint_{\log(4\pi n^{\lambda_\pm})}^{\Omega} \left\{ \left( \frac{\eta_0^{\pm} \cdot \lambda_\pm^2}{2\pi l} \right) \cdot \exp\left(-\lambda_\pm \cdot |\mathfrak{r} - \mathfrak{r}'|\right) \cdot F_\pm(c) \cdot \frac{\partial^{2-n}\boldsymbol{\psi}}{\partial t^{2-n}} \Big( -\mathbb{H}_\pm \cdot |\mathfrak{r} - \mathfrak{r}'|^n \Big) \right\} \mathrm{d}\,\mathbb{H}_{\Omega_n}\, \mathrm{d}\boldsymbol{\psi}_{\Omega_n}$$



## Abstract

The connection between the quantized wave function method and the coordinate-space formulation is examined. The operators of the second quantization are represented in a sequence of configuration spaces for $1, \ldots, 2, \ldots$ etc. particles. The representation obtained enables a simple derivation of HARTREE's equations with exchange.

# List of Symbols

| | |
|---|---|
| $e_0$ | elementary charge, $1.602\,176 \times 10^{-19}$ C |
| $\hbar$ | $= \frac{h}{2\pi}$, mit $h = 6.626 \times 10^{-34}$ J s, PLANCK's constant |
| $\mathfrak{H}$ | energy operator |
| $\mathbb{H}$ | transformed energy operator, see Equation 26 |
| $\mathscr{H}$ | HAMILTON operator |
| $n$ | total number of particles, $n$ particles |
| $\mathtt{m}$ | operator, to which is assigned the number $n$ of particles, see Equation 1 |
| $n_1, n_2, \ldots$ | particle $1, 2, \ldots$ |
| $p, q, r, s$ | summation indices |
| $\boldsymbol{\psi}(x)$ | quantized wave function |
| $\boldsymbol{\psi}^{\dagger}(x)$ | the quantized wave function adjoint to $\boldsymbol{\psi}(x)$ |
| $\psi(x_1, x_2, \ldots, x_n; t)$ | wave function |
| $\mathfrak{r}$ | distance vector |
| $\sigma_r$ | spin coordinate |
| $S(t)$ | unitary operator |
| $S^{\dagger}(t)$ | the unitary operator adjoint to $S(t)$ |
| $t$ | time |
| $\mathsf{V}(\mathfrak{r})$ | operator for the COULOMB potential |
| $x_1, x_2, \ldots, x_n$ | cartesian coordinates of all particles |

## Configuration Space and Second Quantization

The equivalence of the method of quantized wave functions with that of ordinary wave functions in configuration space is known in principle; however, it appears that the closer relationship between the two methods has not received sufficient attention. In the present work, the relationship between the two methods is pursued in detail. It turns out that this relationship is so close that one can move directly to the configuration space at any stage of the calculation with quantized wave functions.

The work contains two parts. The *first* part has an introductory character and contains a derivation and compilation of known results. The transition from configuration space to second quantization is considered there for the case of Bose and Fermi statistics, whereby the uniqueness of the determination of the order of non-interchangeable factors is especially pointed out. The starting point for the considerations in the *second part* are the commutation relations between the quantized wave functions ($\boldsymbol{\psi}$ operators). It is shown that these relations are satisfied by certain operators acting on a sequence of ordinary wave functions for $1, 2, \ldots, n, \ldots$ particles. Through this the $\boldsymbol{\psi}$ operators are represented in the configuration space (more precisely: in a sequence of configuration spaces). Furthermore, the dependence of the $\boldsymbol{\psi}$ operators on time is considered and the form of the operator $\dot{\boldsymbol{\psi}} = \frac{\partial \boldsymbol{\psi}}{\partial t}$ is found. Based on the obtained representation it is shown that the time-dependent Schrödinger equation for the $\boldsymbol{\psi}$ operators can be written as a sequence of ordinary Schrödinger equations for $1, 2, \ldots, n \ldots$ particles. As a further application of the representation obtained, a simple derivation of Hartree's equations with exchange is given.

# 1 Part I – Transition from configuration space to second quantization

The reader who is familiar with the theory of second quantization can skip this first part and start reading straight away with the second part, see section 2. Relevant literature can be found in [1, 8, 6, 5, 9]

We denote by $x_r$ the totality of the variables of the $r$-th particle (e.g. the coordinates and the spin of the electron, $x_r = (x_r, y_r, z_r, \sigma_r)$) and consider the wave function

$$\psi\left(x_1, x_2, \ldots, x_n; t\right) , \tag{1}$$

which describes the entirety of $n$ identical particles in the configuration space. It is convenient to move from the original variables $x$ to new variables $E$ with only discrete values

$$E = E^{(1)}, E^{(2)}, \ldots, E^{(r)}, \ldots \tag{2}$$

through a canonical transformation; The quantities according to Equation 2 can be thought of as eigenvalues of an operator with a discrete spectrum. If we denote the corresponding eigenfunctions by

$$\psi_r(x) = \psi\left(E^{(r)}, x\right) , \tag{3}$$

the transformed wave function

$$c\left(E_1, E_2, \ldots, E_n; t\right) \tag{4}$$

is linked to the original wave function according to Equation 1 by the relation

$$\psi\left(x_1, x_2, \ldots, x_n; t\right) = \sum_{E_1,\ldots,E_n} c\left(E_1, E_2, \ldots, E_n; t\right) \cdot \psi\left(E_1; x_1\right) \ldots \psi\left(E_n; x_n\right) ; \tag{5}$$

where each of the summation variables $E_1, E_2, \ldots, E_n$ passes through all values of Equation 2.
The Schrödinger equation in configuration space is given by[2]

$$\mathfrak{H}\,\psi\left(x_1, x_2, \ldots, x_n; t\right) - \mathtt{i}\,\hbar \cdot \frac{\partial \psi}{\partial t} = 0\,. \tag{6}$$

We assume that the energy operator $\mathfrak{H}$ is of the following form:

$$\mathfrak{H} = \sum_{k=1}^{n} H\left(x_k\right) + \sum_{k<l=1}^{n} G\left(x_k, x_l\right) . \tag{7}$$

[2]Here, $\hbar$ denotes Planck's constant divided by $2\pi$; $\hbar = \frac{h}{2\pi}$

The simple sum describes the energy of the individual particles, the double sum describes their interaction energy. In the case of Coulomb forces

$$G\left(x, x'\right) = \frac{e_0^2}{|\mathfrak{r} - \mathfrak{r}'|} \tag{8}$$

applies. The Schrödinger equation for the transformed wave functions according to Equation 4 is obtained by introducing Equation 5 into Equation 6, and expanding the result according to the products

$$\psi\left(E_1; x_1\right), \ldots, \psi\left(E_n; x_n\right)$$

of the functions according to Equation 3 and setting the coefficients of the individual products equal to zero. There results

$$\begin{aligned}
&\sum_{k=1}^{n} \sum_{W} \left(E_k|H|W\right) \cdot c\left(E_1, \ldots, E_{k-1}, W, E_{k+1}, \ldots, E_n; t\right) \\
&+ \sum_{k<l=1}^{n} \sum_{WW'} \left(E_k E_l|G|WW'\right) \\
&\cdot\ c\left(E_1, \ldots, E_{k-1}, W, E_{k+1}, \ldots, E_{l-1}, W', E_{l+1}, \ldots, E_n; t\right) \\
&- \mathrm{i}\, \hbar \cdot \frac{\partial}{\partial t} c\left(E_1, \ldots, E_n; t\right) = 0\,,
\end{aligned} \tag{9}$$

where the following designations for the matrix elements were introduced:

$$\left(E|H|W\right) = \int \overline{\psi}(E; x) \cdot H(x) \cdot \psi(W; x)\, \mathrm{d}x\,, \tag{10a}$$

$$\begin{aligned}
\left(EE'|G|WW'\right) = &\iint \overline{\psi}(E; x) \cdot \overline{\psi}\left(E'; x'\right) \\
&\cdot\ G\left(x, x'\right) \cdot \psi(W; x) \cdot \psi\left(W'; x'\right) \mathrm{d}x\, \mathrm{d}x'\,.
\end{aligned} \tag{10b}$$

The arguments

$$E_1, E_2, \ldots, E_k, \ldots, E_n$$

of the wave function $c$ in Equation 9 may be correspondingly equal to the eigenvalues

$$E^{(r_1)}, E^{(r_2)}, \ldots, E^{(r_k)}, \ldots, E^{(r_n)}\,.$$

If we write for abbreviation

$$\begin{gathered}
(r|H|s) \text{ instead of } \left(E^{(r)}|H|E^{(s)}\right)\,, \\
(rt|G|su) \text{ instead of } \left(E^{(r)}E^{(t)}|G|E^{(s)}E^{(u)}\right)\,, \\
c\left(r_1, r_2, \ldots, r_n; t\right) \text{ instead of } c\left(E^{(r_1)}, E^{(r_2)}, \ldots, E^{(r_n)}; t\right)\,,
\end{gathered}$$

then the wave equation becomes equal to

$$\boxed{\begin{aligned}&\sum_r \sum_{k=1}^{n} (r_k|H|r)\, c\,(r_1,\ldots,r_{k-1},r,r_{k+1},\ldots,r_n;t)\\&+\sum_{rs}\sum_{k<l=1}^{n}(r_k r_l|G|rs)\\&\cdot c\,(r_1,\ldots,r_{k-1},r,r_{k+1},\ldots,r_{l-1},s,r_{l+1},\ldots,r_n;t)\\&-\mathtt{i}\,\hbar\cdot\frac{\partial}{\partial t}c\,(r_1,\ldots,r_n;t)=0\end{aligned}} \tag{9a}$$

according to Equation 9.

So far we have not considered the symmetry properties of the wave function, i.e. the type of statistics. Now the wave function (both $\psi$ and $c$) is either symmetric (Bose Statistics) or antisymmetric (Fermi Statistics). In the case of the symmetric wave function, fixing the numbers

$$n_1, n_2, \ldots, n_r, \ldots \tag{11}$$

is sufficient to determine the value of $c(r_1, r_2, \ldots, r_n; t)$[3], which indicate how often the argument

$$1, 2, \ldots, r, \ldots$$

or

$$E^{(1)}, E^{(2)}, \ldots, E^{(r)}, \ldots$$

in question occurs in $c$. We can therefore put:

$$c(r_1, r_2, \ldots, r_n; t) = c^\star(n_1, n_2, \ldots; t)\,. \tag{12}$$

A specific sequence of numbers according to Equation 11 now corresponds to a specific system of values $r_1, r_2, \ldots, r_n$ regardless of the order of the latter quantities. For example, we have (for $n = 3$)

$$c(4,4,5) = c(4,5,4) = c(5,4,4) = c^\star(0,0,0,2,1,0,0,\ldots)\,.$$

In the normalization condition

$$\sum_{r_1,\ldots,r_n} |c\,(r_1, r_2, \ldots, r_n; t)|^2 = 1 \tag{13}$$

one can first carry out the summation over all permutations of the numbers of a fixed system of values $r_1, r_2, \ldots, r_n$ and then over different systems of values:

$$\sum_{(r_1,\ldots,r_n)} \sum_{\text{Perm.}} |c\,(r_1, r_2, \ldots, r_n; t)|^2 = 1\,.$$

[3]In the infinite sequence of numbers according to Equation 11 there are at most $n$ numbers other than zero.

The sum $\sum_{\text{Perm.}}$ contains $\frac{n!}{n_1!\cdot n_2!\cdot\ldots}$ equal terms; we therefore have

$$\sum_{(r_1,\ldots,r_n)} \frac{n!}{n_1!\cdot n_2!\cdot\ldots}\cdot\left|c\left(r_1,r_2,\ldots,r_n;t\right)\right|^2 = 1$$

or, if we introduce the $n_r$ as a variable according to Equation 12

$$\sum_{n_1,n_2,\ldots} \frac{n!}{n_1!\cdot n_2!\cdot\ldots}\cdot\left|c^\star\left(n_1,n_2,\ldots;t\right)\right|^2 = 1\,. \tag{14}$$

In the normalization condition according to Equation 14 the "density function" $\frac{n!}{n_1!\cdot n_2!\cdot\ldots}$ can be reduced to 1 through the Ansatz[4]

$$c^\star\left(n_1,n_2,\ldots;t\right) = \sqrt{\frac{n_1!\cdot n_2!\cdot\ldots}{n!}}\cdot f\left(n_1,n_2,\ldots;t\right)\,. \tag{15}$$

For the new wave function $f$ the normalization condition then follows as

$$\sum_{n_1,n_2,\ldots}\left|f\left(n_1,n_2,\ldots;t\right)\right|^2 = 1\,. \tag{16}$$

In the case of Fermi Statistics, specifying the numbers $n_r$ is not initially sufficient to clearly determine $c\left(r_1,r_2,\ldots;t\right)$, because this specification means that the quantity $c$ is only determined up to the sign. But we can also retain Equation 12 and Equation 15 for the Fermi Statistics if we introduce the additional condition that the arguments in $c\left(r_1,r_2,\ldots;t\right)$ should form a "natural" order, e.g.

$$r_1 < r_2 < r_3\cdots < r_n\,.$$

If the order of the arguments arises from the natural one by an even permutation, Equation 12 holds unchanged; for an odd permutation the sign must be changed. We have e.g.

$$c(1,4,5) = -c(4,1,5) = c^\star(1,0,0,1,1,0,0,\ldots)\,.$$

From now on we will consider the Bose and Fermi Statistics separately.

[4]For the definition of an "Ansatz", see e.g. `https://en.wikipedia.org/wiki/Ansatz`

## 1.1 Bose Statistics

In the case of Bose Statistics, several identical arguments can occur in the wave function $c\,(r_1, r_2, \ldots; t)$, e.g.

$$c = c(u, u, u, v, v, w, \ldots)\,.$$

In the first sum of the expression according to Equation 9a, functions can therefore occur that only differ in the order of the arguments, namely there are $n_u$ terms in which the argument $r$ takes the place of $u$, $n_v$ terms with $r$ instead of $v$, etc. If we combine the same terms, we get the expression

$$\begin{aligned}&\sum_r (u|H|r)\, n_u \cdot c(r, u, u, v, v, w, \ldots)\\ &+ \sum_r (v|H|r)\, n_v \cdot c(u, u, u, r, v, w, \ldots)\\ &+ \cdots\end{aligned}$$

for the first sum in Equation 9a. If we introduce $n_k$ as a variable here according to Equation 12, we get

$$\begin{aligned}&\sum_r (u|H|r)\, n_u \cdot c^\star\,(\ldots, n_u - 1, \ldots, n_r + 1, \ldots)\\ &+ \sum_r (v|H|r)\, n_v \cdot c^\star\,(\ldots, n_v - 1, \ldots, n_r + 1, \ldots)\\ &+ \cdots\end{aligned}$$

or more simply

$$\sum_p \sum_r (p|H|r)\, n_p \cdot c^\star \Big(\ldots, n_p - 1, \ldots, n_r + 1, \ldots\Big)\,, \tag{17}$$

where the index $p$ now can pass through *all* values (and not just the values $p = u, v, w, \ldots$), since the superfluous terms disappear because of the factor $n_p$. For $r = p$,

$$c^\star \Big(\ldots, n_p - 1, \ldots, n_r + 1, \ldots\Big)$$

simply means

$$c^\star\,(\ldots, n_r, \ldots)\,.$$

Analogously one can also transform the second sum of the expression in Equation 9a. If we take into account the number of identical terms, we get:

$$\begin{aligned}\sum_{r,s} \Bigg\{&(uu|G|rs) \cdot \frac{1}{2} n_u \cdot (n_u - 1) \cdot c(r, s, u, v, v, w, \ldots)\\ &+ (uv|G|rs) \cdot n_u n_v \cdot c(r, u, u, s, v, w, \ldots)\\ &+ (vv|G|rs) \cdot \frac{1}{2} n_v \cdot (n_v - 1) \cdot c(u, u, u, r, s, w, \ldots) + \cdots \Bigg\}\,,\end{aligned}$$

and if we introduce the quantities $c^\star(n_1, n_2, \ldots)$:

$$\sum_{r,s} \Big\{ (uu|G|rs) \cdot \frac{1}{2} n_u \cdot (n_u - 1) \cdot c^\star(\ldots, n_u - 2, \ldots, n_r + 1, \ldots, n_s + 1, \ldots)$$
$$+ (uv|G|rs) \cdot n_u n_v \cdot c^\star(\ldots, n_u - 1, \ldots, n_v - 1, \ldots, n_r + 1, \ldots, n_s + 1, \ldots)$$
$$+ (vv|G|rs) \cdot \frac{1}{2} n_v \cdot (n_v - 1) \cdot c^\star(\ldots, n_v - 2, \ldots, n_r + 1, \ldots, n_s + 1, \ldots)$$
$$+ \cdots \Big\}$$

or more simply

$$\frac{1}{2} \cdot \sum_{p,q} \sum_{r,s} (pq|G|rs) \cdot n_p \cdot \left(n_q - \delta_{pq}\right) \cdot c^\star\left(\ldots, n_p - 1, \ldots, n_q - 1, \ldots, n_r + 1, \ldots, n_s + 1, \ldots\right). \tag{18}$$

Here again the summation indices $p$ and $q$ can pass through all values without exception (and not just $p, q = u, v, w, \ldots$). The factor $1/2$ must be present in *all* terms, since, for example, both the combination $p = u$ and $q = v$ as well as $p = v$ and $q = u$ occurs in Equation 18. The meaning of the term in Equation 18 for the case that two or more of the numbers $p$, $q$, $r$, $s$ coincide probably does not require any special explanation.

Using Equation 17 and Equation 18, the wave equation according to Equation 9a can be written as:

$$\left.\begin{aligned}
&\sum_p \sum_r (p|H|r) \cdot n_p \cdot c^\star\left(\ldots, n_p - 1, \ldots, n_r + 1, \ldots\right) \\
&+ \frac{1}{2} \cdot \sum_{pq} \sum_{rs} (pq|G|rs) \cdot n_p \cdot \left(n_q - \delta_{pq}\right) \\
&\cdot c^\star\left(\ldots, n_p - 1, \ldots, n_q - 1, \ldots, n_r + 1, \ldots, n_s + 1, \ldots\right) \\
&- \mathrm{i}\,\hbar \cdot \frac{\partial}{\partial t} c^\star(n_1, n_2, \ldots; t) = 0\,.
\end{aligned}\right\} \tag{19}$$

To proceed further, it is convenient to introduce the operator $U_r$, which transforms a function

$$f(n_1, n_2, \ldots, n_r, \ldots)$$

into

$$f(n_1, n_2, \ldots, n_r + 1, \ldots)$$

according to

$$U_r \cdot f(n_1, n_2, \ldots, n_r, \ldots) = f(n_1, n_2, \ldots, n_r + 1, \ldots)\,. \tag{20}$$

The matrix of $U_r$ and its adjoint $U_r^\dagger$ are of the form

$$U_r = \left\{\begin{matrix} 0 & 1 & 0 & 0 & \vdots \\ 0 & 0 & 1 & 0 & \vdots \\ 0 & 0 & 0 & 1 & \vdots \\ 0 & 0 & 0 & 0 & \vdots \\ \dots & \dots & \dots & \dots & \end{matrix}\right\} ; \; U_r^\dagger = \left\{\begin{matrix} 0 & 0 & 0 & 0 & \vdots \\ 1 & 0 & 0 & 0 & \vdots \\ 0 & 1 & 0 & 0 & \vdots \\ 0 & 0 & 1 & 0 & \vdots \\ \dots & \dots & \dots & \dots & \end{matrix}\right\} \tag{21}$$

with respect to the variable $n_r$. Consequently, the adjoint operator $U_r^\dagger$ transforms the function $f(n_1, n_2, \dots, n_r, \dots)$ into $f(n_1, n_2, \dots, n_r - 1 \dots)$ if $n_r \neq 0$ and into 0 for $n_r = 0$. So

$$\left.\begin{aligned} U_r^\dagger f(n_1, n_2, \dots, n_r, \dots) &= f(n_1, n_2, \dots, n_r - 1, \dots) \quad (n_r \neq 0) \\ &= 0 \qquad\qquad\qquad\qquad\qquad\qquad (n_r = 0) \end{aligned}\right\} \tag{22}$$

From the definition of $U_r$ it follows

$$U_r^\dagger \cdot U_r = 1\,. \tag{23a}$$

On the other hand, $U_r \cdot U_r^\dagger \neq 1$, namely

$$U_r \cdot U_r^\dagger = \left\{\begin{matrix} 0 & 0 & 0 & 0 & \vdots \\ 0 & 1 & 0 & 0 & \vdots \\ 0 & 0 & 1 & 0 & \vdots \\ 0 & 0 & 0 & 1 & \vdots \\ \dots & \dots & \dots & \dots & \end{matrix}\right\} . \tag{23b}$$

So the operator $U_r$ is not unitary.

Furthermore, for $p \neq r$ $U_p$ and $U_p^\dagger$ are interchangeable with $U_r$ and $U_r^\dagger$.

Using the operators $U_p$, the functions $c^\star$ appearing in Equation 19 can be written in the following form:

$$\begin{aligned} c^\star\left(\dots, n_p - 1, \dots, n_r + 1, \dots\right) &= U_p^\dagger U_r \cdot c^\star\left(\dots, n_p, \dots, n_r, \dots\right) , \\ c^\star\left(\dots, n_p - 1, \dots, n_q - 1, \dots, n_r + 1, \dots, n_s + 1, \dots\right) & \\ = U_p^\dagger U_q^\dagger U_s U_r \cdot c^\star\left(n_1, n_2, \dots, n_p, \dots, n_q, \dots, n_r, \dots, n_s, \dots\right) . & \end{aligned}$$

The order of the factors ($U^\dagger$ to the left of $U$) follows clearly from the definition of $c^\star$ for $p = r$ in conjunction with Equation 23a and Equation 23b. These expressions apply to

arbitrary (even coincident) values of $p$, $q$, $r$, $s$. If one introduces them into Equation 19, one gets

$$\begin{aligned}
&\sum_p \sum_q (p|H|r) \cdot n_p U_p^\dagger U_r \cdot c^\star(n_1, n_2, \ldots) \\
+\frac{1}{2} \cdot &\sum_{pq} \sum_{rs} (pq|G|rs) \cdot n_p \cdot \left(n_q - \delta_{pq}\right) \cdot U_p^\dagger U_q^\dagger U_s U_r \cdot c^\star(n_1, n_2, \ldots) \\
&- \mathtt{i}\,\hbar \cdot \frac{\partial}{\partial t} c^\star(n_1, n_2, \ldots; t) = 0\,. \qquad (19a)
\end{aligned}$$

Here we still have to express $c^\star(n_1, n_2, \ldots)$ according to Equation 15 by $f(n_1, n_2, \ldots)$. The operator $n$ for the total number of particles, and consequently also $n!$, apparently commutes with the products $U_p^\dagger \cdot U_r$ and $U_p^\dagger \cdot U_q^\dagger \cdot U_r \cdot U_s$; further we have

$$\frac{1}{\sqrt{n_1! \cdot n_2! \cdot \ldots}} \cdot U_r \cdot \sqrt{n_1! \cdot n_2! \cdot \ldots} = \sqrt{n_r + 1} \cdot U_r = U_r \cdot \sqrt{n_r}\,, \qquad (24a)$$

$$\frac{1}{\sqrt{n_1! \cdot n_2! \cdot \ldots}} \cdot U_r^\dagger \cdot \sqrt{n_1! \cdot n_2! \cdot \ldots} = \frac{1}{\sqrt{n_r}} \cdot U_r^\dagger\,. \qquad (24b)$$

The one with $\sqrt{\frac{n!}{n_1! \cdot n_2! \cdot \ldots}}$ multiplied term $n_p U_p^\dagger U_r c^\star(n_1, n_2, \ldots)$ of the first sum in Equation 19a is therefore equal to

$$\begin{aligned}
&\sqrt{\frac{n!}{n_1! \cdot n_2! \cdot \ldots}} \cdot n_p U_p^\dagger U_r \cdot \sqrt{\frac{n_1! \cdot n_2! \cdot \ldots}{n!}} \cdot f(n_1, n_2, \ldots) \\
&= \sqrt{n_p} \cdot U_p^\dagger U_r \cdot \sqrt{n_r} \cdot f(n_1, n_2, \ldots)\,.
\end{aligned}$$

Analogously, using Equation 24a and Equation 24b and the relation

$$\left(n_q - \delta_{pq}\right) \cdot U_p^\dagger = U_p^\dagger n_q$$

for a term of the second sum in Equation 19a, we obtain the expression

$$\begin{aligned}
&\sqrt{\frac{n!}{n_1! \cdot n_2! \cdot \ldots}} \cdot n_p \cdot \left(n_q - \delta_{pq}\right) \cdot U_p^\dagger U_q U_s U_r \cdot \sqrt{\frac{n_1! \cdot n_2! \cdot \ldots}{n!}} \cdot f(n_1, n_2, \ldots) \\
&= \sqrt{n_p} \cdot U_p^\dagger \cdot \sqrt{n_q} \cdot U_q^\dagger \cdot U_s \cdot \sqrt{n_s} \cdot U_r \cdot \sqrt{n_r} \cdot f(n_1, n_2, \ldots)\,.
\end{aligned}$$

If one introduces these expressions into Equation 19a, one obtains for $f(n_1, n_2, \ldots; t)$ the wave equation

$$\mathbb{H}\, f(n_1, n_2, \ldots; t) - \mathtt{i}\,\hbar \cdot \frac{\partial f}{\partial t} = 0\,, \qquad (25)$$

where $\mathbb{H}$ denotes the transformed energy operator

$$\begin{aligned}
\mathbb{H} = &\sum_{pr} (p|H|r) \cdot \sqrt{n_p} U_p^\dagger U_r \sqrt{n_r} \\
&+ \frac{1}{2} \cdot \sum_{pqrs} (pq|G|rs) \cdot \sqrt{n_p} U_p^\dagger \sqrt{n_q} U_q^\dagger U_s \sqrt{n_s} U_r \sqrt{n_r}\,. \qquad (26)
\end{aligned}$$

The operators $U_r$ and $n_r$ only appear here in the combination

$$\left.\begin{aligned} b_r &= U_r \cdot \sqrt{n_r}\,, \\ b_r^\dagger &= \sqrt{n_r} \cdot U_r^\dagger\,. \end{aligned}\right\} \tag{27}$$

If one introduces Equation 27 into Equation 26, one gets the following expression for $\mathbb{H}$:

$$\mathbb{H} = \sum_{pr} b_p^\dagger\,(p|H|r)\,b_r + \frac{1}{2} \cdot \sum_{pqrs} b_p^\dagger b_q^\dagger\,(pq|G|rs)\,b_s b_r\,. \tag{28}$$

As can be seen from the definition according to Equation 20 and Equation 22 of $U_r$ and $U_r^\dagger$, the just introduced operators $b_r$ satisfy the relations

$$\left.\begin{aligned} b_r^\dagger \cdot b_r &= n_r \\ b_r \cdot b_r^\dagger &= n_r + 1\,, \end{aligned}\right\} \tag{29}$$

and furthermore, for $r \neq s$ the $b_r$ and $b_r^\dagger$ are interchangeable with $b_s$ and $b_s^\dagger$, then one has the well-known interchange relations

$$b_r \cdot b_s^\dagger - b_s^\dagger \cdot b_r = \delta_{rs}\,, \tag{30a}$$

$$b_r \cdot b_s - b_s \cdot b_r = 0\,. \tag{30b}$$

If one now uses $b_r$ to form the quantized wave function

$$\boldsymbol{\psi}(x) = \sum_r b_r \cdot \psi_r(x) \tag{31a}$$

with its adjoint

$$\boldsymbol{\psi}^\dagger(x) = \sum_r b_r^\dagger \cdot \overline{\psi}_r(x)\,, \tag{31b}$$

the energy operator $\mathbb{H}$ can be represented in the following form:

$$\begin{aligned} \mathbb{H} = &\int \boldsymbol{\psi}^\dagger(x) \cdot H(x) \cdot \boldsymbol{\psi}(x)\,\mathrm{d}x \\ &+ \frac{1}{2} \cdot \iint \boldsymbol{\psi}^\dagger(x) \cdot \boldsymbol{\psi}^\dagger(x') \cdot G(x,x') \cdot \boldsymbol{\psi}(x') \cdot \boldsymbol{\psi}(x)\,\mathrm{d}x\,\mathrm{d}x'\,. \end{aligned} \tag{32}$$

The commutation relations for the quantized wave functions ($\boldsymbol{\psi}$ operators) follow easily from Equation 30a and Equation 30b taking into account the equation

$$\sum_r \overline{\psi}_r(x) \cdot \psi_r(x') = \delta\left(x - x'\right)\,.$$

One obtains the expression

$$\boldsymbol{\psi}(x') \cdot \boldsymbol{\psi}^\dagger(x) - \boldsymbol{\psi}^\dagger(x) \cdot \boldsymbol{\psi}(x') = \delta(x - x')\,, \tag{33a}$$

$$\boldsymbol{\psi}(x') \cdot \boldsymbol{\psi}(x) - \boldsymbol{\psi}(x) \cdot \boldsymbol{\psi}(x') = 0\,. \tag{33b}$$

## 1.2 Fermi Statistics

We return to the wave equation Equation 9a. We think of the numbers $r_1, r_2, r_3, \ldots$ ordered in the natural order

$$r_1 < r_2 < r_3 < \cdots < r_n \,, \tag{34}$$

so that we have according to Equation 12

$$c\left(r_1, r_2, \ldots, r_n; t\right) = c^\star\left(n_1, n_2, \ldots; t\right) \,. \tag{35}$$

In the natural order, the number $r_k$ is at position

$$k = n_1 + n_2 + \cdots + n_{r_k} \,. \tag{36}$$

In the $k$-th term of the first sum in Equation 9a $r_k$ is replaced by $r$, so that the arguments in $c$ are there in the order

$$r_1, r_2, \ldots, r_{k-1}, r, r_{k+1}, \ldots, r_n \,, \tag{*}$$

which is no longer a natural one: Here $r$ is at position $k$, while it should be at position

$$k' = n_1' + n_2' + \cdots + n_r' \,.$$

(The deleted quantities are the new values of the $n_s$, which correspond to the arguments according to Equation * in $c$.) Therefore it is

$$c\left(r_1, \ldots, r_{k-1}, r, r_{k+1}, \ldots, r_n; t\right) = (-1)^{k+k'} \cdot c^\star\left(\ldots, n_{r_k} - 1, \ldots, n_r + 1, \ldots\right) \,.$$

It is useful at this point to introduce the operators $\alpha_r$ and $\alpha_r^\dagger$ by setting

$$\alpha_r \cdot f\left(n_1, \ldots, n_r, \ldots\right) = \begin{cases} f\left(n_1, \ldots, n_r + 1, \ldots\right) & \text{for } \; n_r = 0 \,, \\ 0 & \text{for } \; n_r = 1 \,, \end{cases} \tag{37a}$$

$$\alpha_r^\dagger \cdot f\left(n_1, \ldots, n_r, \ldots\right) = \begin{cases} 0 & \text{for } \; n_r = 0 \,, \\ f\left(n_1, \ldots, n_r - 1, \ldots\right) & \text{for } \; n_r = 1 \,. \end{cases} \tag{37b}$$

From this definition it follows that for $r \neq s$ the operators $\alpha_r$ and $\alpha_r^\dagger$ are interchangeable with $\alpha_s$ and $\alpha_s^\dagger$ (since they act on different variables) , while for $r = s$ the equations

$$\left.\begin{aligned} \alpha_r^\dagger \cdot \alpha_r &= n_r \,, \\ \alpha_r \cdot \alpha_r^\dagger &= 1 - n_r \end{aligned}\right\} \tag{38}$$

hold. Furthermore, one can easily prove the equation

$$\alpha_r \cdot \left(1 - 2n_r\right) = -\left(1 - 2n_r\right) \cdot \alpha_r \,. \tag{39}$$

Using the operators $\alpha_r$ one can write

$$c^{\star}\left(\ldots, n_{r_k}-1, \ldots, n_r+1, \ldots\right)=\alpha_{r_k}^{\dagger} \alpha_r \cdot c^{\star}\left(n_1, n_2, \ldots\right) .$$

The order of the factors $\alpha_{r_k}^{\dagger}$ and $\alpha_k$ is clearly determined here, because for $r = r_k$ and $n_{r_k} = 1$ the factor of $c^{\star}$ on the right must reduce to 1. We have

$$(-1)^k=(-1)^{n_1+\cdots+n_{r_k}}$$

and since for $n = 0$ and $n = 1$ the quantity $(-1)^n$ agrees with $(1 - 2n)$, we can also write for it:

$$(-1)^k=\prod_{p=1}^{r_k}\left(1-2 n_p\right)=\nu_{r_k},$$

where

$$\nu_s=\prod_{p=1}^{s}\left(1-2 n_p\right) \tag{40}$$

is the Wigner' sign function. Analogously,

$$(-1)^{k'}=\nu_r',$$

where $\nu_r'$ is formed with the numbers $n_r'$. So we have

$$c\left(r_1, r_2, \ldots, r_{k-1}, r, r_{k+1}, \ldots ; t\right)=\nu_{r_k} \nu_r' \alpha_{r_k}^{\dagger} \alpha_r \cdot c^{\star}\left(n_1, n_2, \ldots\right),$$

and because of

$$\nu_r' \alpha_{r_k}^{\dagger} \alpha_r=\alpha_{r_k}^{\dagger} \alpha_r \nu_r$$

we can write for it:

$$c\left(r_1, r, \ldots, r_{k-1}, r, r_{k+1}, \ldots ; t\right)=\nu_{r_k} \alpha_{r_k}^{\dagger} \alpha_r \nu_r \cdot c^{\star}\left(n_1, n_2, \ldots\right) .$$

The first sum in Equation 9a is therefore equal to

$$\sum_r \sum_{k=1}^{n}\left(r_k|H| r\right) \cdot \nu_{r_k} \alpha_{r_k}^{\dagger} \alpha_r \nu_r \cdot c^{\star}\left(n_1, n_2, \ldots\right) .$$

When summing over $k$, the index $r_k$ runs through the values $r_k = r_1, r_2, \ldots, r_n$. Instead, one can let $r_k$ pass through *all* values, because the superfluous terms disappear due to the property of the operator $\alpha^{\dagger}$. So we get the expression

$$\sum_p \sum_r (p|H| r)\, \nu_p \alpha_p^{\dagger} \alpha_r \nu_r \cdot c^{\star}\left(n_1, n_2, \ldots\right) \tag{41}$$

for the sum under consideration. We now want to transform the second sum in Equation 9a. Above all, it is about determining the sign in the equation

$$\begin{aligned}
&\pm c\,(r_1,\dots,r_{k-1},r,r_{k+1},\dots,r_{l-1},s,r_{l+1},\dots,r_n;t)\\
&= c^\star\,(\dots,n_{r_k}-1,\dots,n_{r_l}-1,\dots,n_r+1,\dots,n_s+1,\dots)\\
&= c^\star\,(n_1',n_2',\dots)\ .
\end{aligned}$$

We first transfer the argument $r$, which is in the $k$-th position, to the first position in $c$; This gives $c$ the factor $-(-1)^k = -\nu_{r_k}$ and we have

$$\begin{aligned}
&c\,(r_1,\dots,r_{k-1},r,r_{k+1},\dots,r_{l-1},s,r_{l+1},\dots,r_n;t)\\
&= -\nu_{r_k}\cdot c\,(r,r_1,\dots,r_{k-1},r_{k+1},\dots,r_{l-1},s,r_{l+1},\dots,r_n;t)\ .
\end{aligned}$$

If $r_l > r_k$, $s$ remained at position

$$l = n_1 + n_2 + \cdots n_{r_l}\,;$$

for $r_l < r_k$, however, $s$ has moved one place to the right and is now at position $l+1$. If we now transfer $s$ to the second position, we get

$$c\,(\dots,r_{k-1},r,r_{k+1},\dots,r_{l-1},s,r_{l+1},\dots) = \begin{cases} -\nu_{r_k}\nu_{r_l}c\,(r,s,r_1,r_2,\dots) & \text{for } r_l > r_k\,,\\ +\nu_{r_k}\nu_{r_l}c\,(r,s,r_1,r_2,\dots) & \text{for } r_l < r_k\,. \end{cases}$$

On the other hand, if we now denote the natural positions of $r$ and $s$ by $k'$ and $l'$ according to

$$\begin{aligned}
k' &= n_1' + n_2' + \cdots + n_r'\,,\\
l' &= n_1' + n_2' + \cdots + n_s'\,,
\end{aligned}$$

we get

$$c\,\overbrace{(\dots,r_1,\dots,r,\dots,s,\dots)}^{\text{natural order}} = c^\star\,(n_1',n_2',\dots) = \begin{cases} -\nu_r'\nu_s'c\,(r,s,r_1,r_2,\dots) & \text{for } s > r\,,\\ +\nu_r'\nu_s'c\,(r,s,r_1,r_2,\dots) & \text{for } s < r \end{cases}$$

by a completely analogous consideration. Together with the previous equation, this gives

$$\begin{aligned}
&c\,(\dots,r_{k-1},r,r_{k+1},\dots,r_{l-1},s,r_{l+1},\dots)\\
&= \begin{cases} +\nu_{r_k}\nu_{r_l}\nu_r'\nu_s'c^\star\left(n_1',n_2',\dots\right) & \text{in case I}\,,\\ -\nu_{r_k}\nu_{r_l}\nu_r'\nu_s'c^\star\left(n_1',n_2',\dots\right) & \text{in case II}\,, \end{cases}
\end{aligned}$$

where cases I and II are characterized by the inequalities

$$\left.\begin{array}{r} r_l > r_k \text{ and } s > r\\ \text{or}\quad r_l < r_k \text{ and } s < r \end{array}\right\}\ \text{case I,}$$

$$\text{or} \quad \left.\begin{matrix} r_l > r_k \text{ and } s < r \\ r_l < r_k \text{ and } s > r \end{matrix}\right\} \quad \text{case II.}$$

Replacing the arguments $n_1, n_2, \ldots$ with $n'_1, n'_2, \ldots$ in $c^\star$ is caused by the operator $\alpha^\dagger_{r_k}\alpha^\dagger_{r_l}\alpha_s\alpha_r$:

$$c^\star\left(n'_1, n'_2, \ldots\right) = \alpha^\dagger_{r_k}\alpha^\dagger_{r_l}\alpha_s\alpha_r \cdot c^\star\left(n_1, n_2, \ldots\right)$$

One can be convinced that the order of the factors $\alpha^\dagger$ and $\alpha$ (as far as it is important) is chosen correctly by considering the special cases $r = r_k$, $s = r_l$ and $r = r_l$, $s = r_k$. If we also take equation

$$\nu'_r\nu'_s\alpha^\dagger_{r_k}\alpha^\dagger_{r_l}\alpha_s\alpha_r = \alpha^\dagger_{r_k}\alpha^\dagger_{r_l}\alpha_s\alpha_r\nu_r\nu_s$$

into account, we have

$$\begin{aligned} &c\left(\ldots, r_{k-1}, r, r_{k+1}, \ldots, r_{l-1}, s, r_{l+1}, \ldots\right) \\ &= \begin{cases} +\nu_{r_k}\nu_{r_l}\alpha^\dagger_{r_k}\alpha^\dagger_{r_l}\alpha_s\alpha_r\nu_s\nu_r c^\star\left(n_1, n_2, \ldots\right) & \text{in case I,} \\ -\nu_{r_k}\nu_{r_l}\alpha^\dagger_{r_k}\alpha^\dagger_{r_l}\alpha_s\alpha_r\nu_s\nu_r c^\star\left(n_1, n_2, \ldots\right) & \text{in case II.} \end{cases} \end{aligned}$$

Now it follows from Equation 39 and from the definition according to Equation 40 of $\nu_s$

$$\left.\begin{aligned} \alpha_r \cdot \nu_s &= \phantom{-}\nu_s \cdot \alpha_r \text{ for } r > s\,, \\ \alpha_r \cdot \nu_s &= -\nu_s \cdot \alpha_r \text{ for } r \leqslant s\,. \end{aligned}\right\} \tag{42}$$

Therefore, in case I we have either

$$\left.\begin{aligned} &\alpha_r \cdot \nu_s = \nu_s \cdot \alpha_r \\ \text{and} \\ &\alpha^\dagger_{r_k} \cdot \nu_{r_l} = \nu_{r_l} \cdot \alpha^\dagger_{r_k} \end{aligned}\right\} \text{for } r > s \text{ and } r_k > r_l$$

at the same time or

$$\left.\begin{aligned} &\alpha_r \cdot \nu_s = -\nu_s \cdot \alpha_r \\ \text{and} \\ &\alpha^\dagger_{r_k} \cdot \nu_{r_l} = -\nu_{r_l} \cdot \alpha^\dagger_{r_k} \end{aligned}\right\} \text{for } r < s \text{ and } r_k < r_l$$

at the same time. So, in case I, the operator acting on $c^\star\left(n_1, n_2, \ldots\right)$ is equal to

$$+\nu_{r_k}\alpha^\dagger_{r_k}\nu_{r_l}\alpha^\dagger_{r_l}\alpha_s\nu_s\alpha_r\nu_r\,.$$

But this operator also has the same sign in case II, because we then have either

$$\left.\begin{aligned} &\alpha_r \cdot \nu_s = \nu_s \cdot \alpha_r \\ \text{and} \\ &\alpha^\dagger_{r_k} \cdot \nu_{r_l} = -\nu_{r_l} \cdot \alpha^\dagger_{r_k} \end{aligned}\right\} \text{for } r > s \text{ and } r_k < r_l$$

or

$$\left.\begin{aligned} &\alpha_r \cdot \nu_s = -\nu_s \cdot \alpha_r \\ \text{and} \quad & \\ &\alpha_{r_k}^\dagger \cdot \nu_{r_l} = \nu_{r_l} \cdot \alpha_{r_k}^\dagger \end{aligned}\right\} \text{ for } r < s \text{ and } r_k > r_l \,.$$

So we always have

$$c\,(\ldots, r_{k-1}, r, r_{k+1}, \ldots, r_{l-1}, s, r_{l+1}, \ldots) = \nu_{r_k}\alpha_{r_k}^\dagger \nu_{r_l}\alpha_{r_l}^\dagger \alpha_s \nu_s \alpha_r \nu_r \cdot c^\star\,(n_1, n_2, \ldots)\ .$$

We now have to introduce this expression into the second sum in Equation 9a. This sum will be equal to

$$\sum_{rs} \sum_{k<l=1}^{n} (r_k r_l|G|rs) \cdot \nu_{r_k}\alpha_{r_k}^\dagger \nu_{r_l}\alpha_{r_l}^\dagger \alpha_s \nu_s \alpha_r \nu_r \cdot c^\star\,(n_1, n_2, \ldots)\ .$$

If we drop the restriction $k < l$ here, the sum doubles and we have to add the factor $1/2$. We then get

$$\frac{1}{2} \cdot \sum_{pq} \sum_{rs} (pq|G|rs) \cdot \nu_p \alpha_p^\dagger \nu_q \alpha_q^\dagger \alpha_s \nu_s \alpha_r \nu_r \cdot c^\star\,(n_1, n_2, \ldots)\ . \tag{43}$$

Here $p$ and $q$ initially only pass through the values $r_1, r_2, \ldots, r_n$ (where $p \neq q$). But one can let them run through all values without exception if one takes into account that the superfluous terms disappear.

Substituting Equation 35, Equation 41 and Equation 43 into Equation 9a gives the wave equation for the wave function $c^\star\,(n_1, n_2, \ldots; t)$. However, in the case of Fermi Statistics, this wave function differs from the wave function $f\,(n_1, n_2, \ldots)$ according to Equation 15 by only one factor (namely $\sqrt{n!}$), which is interchangeable with the individual terms of the energy operator. Therefore, the wave equation for $f\,(n_1, n_2, \ldots)$ has the same form as for $c^\star\,(n_1, n_2, \ldots)$, namely

$$\mathbb{H}\, f\,(n_1, n_2, \ldots; t) - \mathtt{i}\,\hbar \cdot \frac{\partial f}{\partial t} = 0\,,$$

where the energy operator $\mathbb{H}$ after Equation 41 and Equation 43 has the following form:

$$\mathbb{H} = \sum_{pr} (p|H|r) \cdot \nu_p \alpha_p^\dagger \alpha_r \nu_r + \frac{1}{2} \cdot \sum_{pqrs} (pq|G|rs) \cdot \nu_p \alpha_p^\dagger \nu_q \alpha_q^\dagger \alpha_s \nu_s \alpha_r \nu_r\,. \tag{44}$$

In the energy operator $\mathbb{H}$, the operators $\alpha_r$ and $\nu_r$ only appear in the combination

$$\left.\begin{aligned} a_r &= \alpha_r \cdot \nu_r\,, \\ a_r^\dagger &= \nu_r \cdot \alpha_r^\dagger \end{aligned}\right\} \tag{45}$$

namely

$$\mathbb{H} = \sum_{pr} a_p^\dagger \cdot (p|H|r) \cdot a_r + \frac{1}{2} \cdot \sum_{pqrs} a_p^\dagger a_q^\dagger \cdot (pq|G|rs) \cdot a_s a_r \,. \tag{44a}$$

As can be easily proven with the help of Equation 38 and Equation 42, the "quantized amplitudes" $a_r$ satisfy the equations

$$\left.\begin{aligned} a_r^\dagger \cdot a_r &= n_r \,, \\ a_r \cdot a_r^\dagger &= (1 - n_r) \end{aligned}\right\} \tag{46}$$

and the commutation relations

$$a_r \cdot a_s^\dagger + a_s^\dagger \cdot a_r = \delta_{rs} \,, \tag{47a}$$

$$a_r \cdot a_s + a_s \cdot a_r = 0 \,. \tag{47b}$$

If one uses the "amplitudes" $a_r$ to form the quantized wave functions

$$\boldsymbol{\psi}(x) = \sum_r a_r \cdot \psi_r(x) \,, \tag{48a}$$

$$\boldsymbol{\psi}^\dagger(x) = \sum_r a_r^\dagger \cdot \overline{\psi}_r(x) \,, \tag{48b}$$

which satisfy the commutation relations

$$\boldsymbol{\psi}(x') \cdot \boldsymbol{\psi}^\dagger(x) + \boldsymbol{\psi}^\dagger(x) \cdot \boldsymbol{\psi}(x') = \delta(x - x') \,, \tag{49a}$$

$$\boldsymbol{\psi}(x') \cdot \boldsymbol{\psi}(x) + \boldsymbol{\psi}(x) \cdot \boldsymbol{\psi}(x') = 0 \,, \tag{49b}$$

then one can write the energy operator in the form

$$\begin{aligned} \mathbb{H} = &\int \boldsymbol{\psi}^\dagger(x) \cdot H(x) \cdot \boldsymbol{\psi}(x) \,\mathrm{d}x \\ &+ \frac{1}{2} \cdot \iint \boldsymbol{\psi}^\dagger(x) \cdot \boldsymbol{\psi}^\dagger(x') \cdot G(x, x') \cdot \boldsymbol{\psi}(x') \cdot \boldsymbol{\psi}(x) \,\mathrm{d}x \,\mathrm{d}x' \,, \end{aligned} \tag{50}$$

just as in the case of Bose Statistics.

The transition from the quantized amplitudes $a_r$ (or $b_r$ in the case of Bose Statistics) to the quantized wave functions $\boldsymbol{\psi}(x)$ represents a unitary canonical transformation of the variables of the one particle (Transition from the $E^{(r)}$ according to Equation 2 to the $x$). The $a_r$ (or the $b_r$) can be viewed as quantized wave functions just as well as $\boldsymbol{\psi}(x)$, and the formulæ represented using the $a_r$ (or $b_r$) (like e.g. the commutation relations or the expression for the energy operator) are equivalent in content to those written with the $\boldsymbol{\psi}(x)$.

It should also be noted that all other operators that can be represented in the configuration space can also be transformed according to the pattern of the energy operator and represented using the quantized wave functions. Just as with the energy operator, the order of the non-commutative factors results in an unequivocally clear manner.

# 2 Part II – Representation of the $\psi$ operators in configuration space

In the formulæ of the second quantization, the total number $n$ of particles no longer appears explicitly; the formulæ apply to any or even an indefinite $n$. The number $n$ can be assigned the operator

$$\mathtt{m} = \int \boldsymbol{\psi}^{\dagger}(x) \cdot \boldsymbol{\psi}(x)\, \mathrm{d}x\,, \tag{1}$$

which has the eigenvalues $n = 0, 1, 2, \ldots$

All operators can be divided into two classes with regard to their behavior towards the operator $\mathtt{m}$: the first class includes those that are commutative with $\mathtt{m}$, and the second that includes the non-commutative operators. An independent definition of the operators of the first class is given in the concurrent work by P. Jordan, [7]. It is shown there that all such operators can be constructed by the coordinate-space-method in a form which is completely identical for both statistics; The exact same formulæ even apply to the mathematically possible but physically inconceivable solutions to the many-body problem. It then follows that commutative rules apply to all of these operators, which are independent of the statistics.

Here we want to deal with the representation of the general operators in the configuration space that are not commutative with $\mathtt{m}$; Above all, it is the representation of the operator $\boldsymbol{\psi}(x)$. Of course, the results can also be applied to the operators that are commutative with $\mathtt{m}$, since these can be expressed as $\boldsymbol{\psi}(x)$ and $\boldsymbol{\psi}^{\dagger}(x)$.

In order to capture both types of statistics uniformly, we write the commutation relations for the quantized wave function in the form

$$\boldsymbol{\psi}(x') \cdot \boldsymbol{\psi}^{\dagger}(x) - \varepsilon \cdot \boldsymbol{\psi}^{\dagger}(x) \cdot \boldsymbol{\psi}(x') = \delta\left(x - x'\right)\,, \tag{2a}$$

$$\boldsymbol{\psi}(x') \cdot \boldsymbol{\psi}(x) - \varepsilon \cdot \boldsymbol{\psi}(x) \cdot \boldsymbol{\psi}(x') = 0\,, \tag{2b}$$

where for the Bose Statistics $\varepsilon = +1$ and for the Fermi Statistics $\varepsilon = -1$ is to be set. From the definition according to Equation 1 of the operator $\mathtt{m}$ and from the commutation relations according to Equation 2 it follows that

$$\mathtt{m} \cdot \boldsymbol{\psi} - \boldsymbol{\psi} \cdot (\mathtt{m} - 1) = 0 \tag{3}$$

for both types of statistics. We choose a representation for $\boldsymbol{\psi}(x)$ in which $\mathtt{m}$ has a diagonal form. If we denote the matrix elements of $\boldsymbol{\psi}(x)$ in this representation by $(n|\boldsymbol{\psi}|n')$, it follows from Equation 3 the “selection rule”

$$(n - n' + 1) \cdot (n|\boldsymbol{\psi}|n') = 0\,, \tag{3a}$$

which states that only matrix elements of the form $(n|\boldsymbol{\psi}|n+1)$ are different from zero. The matrix $\boldsymbol{\psi}(x)$ is therefore of the form

$$\boldsymbol{\psi}(x) = \left\{ \begin{array}{ccccc} 0 & (0|\boldsymbol{\psi}|1) & 0 & 0 & \vdots \\ 0 & 0 & (1|\boldsymbol{\psi}|2) & 0 & \vdots \\ 0 & 0 & 0 & (2|\boldsymbol{\psi}|3) & \vdots \\ \cdots & \cdots & \cdots & \cdots & \end{array} \right\} . \tag{4}$$

A single matrix element $(n-1|\boldsymbol{\psi}|n)$ in Equation 4 can be viewed as an operator acting on a function of $n$ variables[5] $x_1, x_2, \ldots, x_n$ and transforming this function into one of $(n-1)$ variables $x_1, x_2, \ldots, x_{n-1}$ and the parameter $x$. So, the operator $\boldsymbol{\psi}(x)$ acts on a sequence of functions

$$\left\{ \begin{array}{c} \text{const.} \\ \psi(x_1) \\ \psi(x_1, x_2) \\ \psi(x_1, x_2, x_3) \\ \cdots\cdots \end{array} \right\} \tag{5}$$

of $0, 1, 2, 3, \ldots$ variables and transforms them into an analog sequence; namely, the functions according to Equation 5 can be understood as ordinary SCHRÖDINGER wave functions in configuration space[6]. We want to say that $\psi(x_1, x_2, \ldots, x_n)$ is the wave function in the "$n$-th subspace". We further want to show that the commutation relations according to Equation 2 are satisfied by the Ansatz

$$(n-1|\boldsymbol{\psi}(x)|n)\, \psi\,(x_1, x_2, \ldots, x_n) = \sqrt{n} \cdot \psi\,(x, x_1, x_2, \ldots, x_{n-1}) \tag{6}$$

if one defines the adjoint operator $\boldsymbol{\psi}^\dagger(x)$ starting from $\boldsymbol{\psi}(x)$ correctly. According to Equation 4 the matrix for $\boldsymbol{\psi}^\dagger(x)$ is of the form

$$\boldsymbol{\psi}^\dagger(x) = \left\{ \begin{array}{cccc} 0 & 0 & 0 & \vdots \\ \left(1|\boldsymbol{\psi}^\dagger|0\right) & 0 & 0 & \vdots \\ 0 & \left(2|\boldsymbol{\psi}^\dagger|1\right) & 0 & \vdots \\ \cdots & \cdots & \cdots & \end{array} \right\} , \tag{4a}$$

where $\left(n|\boldsymbol{\psi}^\dagger(x)|n-1\right)$ is the operator adjoint to $(n-1|\boldsymbol{\psi}(x)|n)$, which transforms a function of $(n-1)$ variables $x_1, x_2, \ldots, x_{n-1}$ into one of $n$ variables $x_1, x_2, \ldots, x_n$ and the parameter $x$. It should be noted that the operator $\left(n|\boldsymbol{\psi}^\dagger(x)|n-1\right)$ must not change the symmetry property of the wave function: it must convert a symmetric function into a symmetric one and convert an antisymmetric into an antisymmetric. We want to find the

[5]Each "Variable" $x_r$ is actually the set of variables, such as $x_r$, $y_r$, $z_r$, $\sigma_r$, which describe the $r$-th particle.
[6]Such function sequences were first considered by L. LANDAU and R. PEIERLS, [10].

operator $\left(n|\boldsymbol{\psi}^{\dagger}(x)|n-1\right)$ by determining its kernel; we can do this if we form the kernel of $(n-1|\boldsymbol{\psi}(x)|n)$ and then move on to the adjoint kernel.

Since the wave function is either symmetric or antisymmetric, one can also write

$$\begin{aligned}&(n-1|\boldsymbol{\psi}(x)|n)\,\psi\,(x_1,x_2,\ldots,x_n)\\ =\;&\frac{1}{\sqrt{n}}\cdot\{\psi\,(x,x_1,x_2,\ldots,x_{n-1})+\varepsilon\cdot\psi\,(x_1,x,x_2,\ldots,x_{n-1})\\ &+\cdots+\varepsilon^{n-1}\cdot\psi\,(x_1,x_2,\ldots,x_{n-1},x)\big\}\end{aligned}\tag{6a}$$

instead of Equation 6. The kernel of the operator defined by Equation 6a is

$$\begin{aligned}&(n-1;x_1,x_2,\ldots,x_{n-1}|\boldsymbol{\psi}(x)|n;\xi_1,\xi_2,\ldots,\xi_n)\\ =\;&\frac{1}{\sqrt{n}}\cdot\big\{\delta\,(\xi_1-x)\cdot\delta\,(\xi_2-x_1)\cdot\ldots\cdot\delta\,(\xi_n-x_{n-1})\\ &+\cdots+\varepsilon^{k-1}\cdot\delta\,(\xi_1-x_1)\cdot\ldots\cdot\delta\,(\xi_{k-1}-x_{k-1})\cdot\delta\,(\xi_k-x)\\ &\cdot\,\delta\,(\xi_{k+1}-x_k)\cdot\ldots\cdot\delta\,(\xi_n-x_{n-1})\\ &+\cdots+\varepsilon^{n-1}\cdot\delta\,(\xi_1-x_1)\cdot\ldots\cdot\delta\,(\xi_{n-1}-x_{n-1})\cdot\delta\,(\xi_n-x)\big\}\,.\end{aligned}\tag{7}$$

The kernel of the adjoint operator $(n|\boldsymbol{\psi}(x)|n-1)$ is obtained by replacing $\xi_1,\xi_2,\ldots,\xi_n$ by $x_1,x_2,\ldots,x_n$ and $x_1,x_2,\ldots,x_{n-1}$ by $\xi_1,\xi_2,\ldots,\xi_{n-1}$ in Equation 7. The result of applying the operator $\left(n|\boldsymbol{\psi}^{\dagger}(x)|n-1\right)$ to the wave function $\psi\,(x_1,x_2,\ldots,x_{n-1})$ is therefore equal to

$$\begin{aligned}&(n|\boldsymbol{\psi}^{+}(x)|n-1)\cdot\psi\,(x_1,x_2,\ldots,x_n)\\ =\;&\frac{1}{\sqrt{n}}\cdot\big\{\delta\,(x_1-x)\cdot\psi\,(x_2,x_3,\ldots,x_n)+\varepsilon\cdot\delta\,(x_2-x)\cdot\psi\,(x_1,x_3,\ldots,x_n)\\ &+\cdots+\varepsilon^{k-1}\cdot\delta\,(x_k-x)\cdot\psi\,(x_1,\ldots,x_{k-1},x_{k+1},\ldots,x_n)\\ &+\cdots+\varepsilon^{n-1}\cdot\delta\,(x_n-x)\cdot\psi\,(x_1,\ldots,x_{n-1})\big\}\,.\end{aligned}\tag{8}$$

The operator $\left(n|\boldsymbol{\psi}^{\dagger}(x)|n-1\right)$ defined by this equation satisfies the requirement that it leaves the symmetry property of the wave function unchanged; the transition from Equation 6 to Equation 6a was carried out precisely for this purpose.

After $\boldsymbol{\psi}(x)$ and $\boldsymbol{\psi}^{\dagger}(x)$ are defined, we can proceed to the proof of the commutation relations according to Equation 2a and Equation 2b. We have to form the operators $\boldsymbol{\psi}^{\dagger}(x)\cdot\boldsymbol{\psi}(x')$ and $\boldsymbol{\psi}(x')\cdot\boldsymbol{\psi}^{\dagger}(x)$. These operators are interchangeable with $\mathtt{m}$, so have diagonal form with respect to $n$. We have

$$\boldsymbol{\psi}^{\dagger}(x)\cdot\boldsymbol{\psi}(x')=\begin{Bmatrix}A_0 & 0 & 0 & \vdots\\ 0 & A_1 & 0 & \vdots\\ 0 & 0 & A_2 & \vdots\\ \cdots & \cdots & \cdots & \end{Bmatrix}\tag{9a}$$

and

$$\boldsymbol{\psi}(x') \cdot \boldsymbol{\psi}^{\dagger}(x) = \begin{Bmatrix} B_0 & 0 & 0 & \vdots \\ 0 & B_1 & 0 & \vdots \\ 0 & 0 & B_2 & \vdots \\ \cdots & \cdots & \cdots & \end{Bmatrix} , \tag{9b}$$

where $A_n$ and $B_n$ denote the operators

$$A_n = \left(n|\boldsymbol{\psi}^{\dagger}(x) \cdot \boldsymbol{\psi}(x')|n\right) = \left(n|\boldsymbol{\psi}^{\dagger}(x)|n-1\right) \cdot (n-1|\boldsymbol{\psi}(x')|n) \tag{10a}$$

and

$$B_n = \left(n|\boldsymbol{\psi}(x') \cdot \boldsymbol{\psi}^{\dagger}(x)|n\right) = (n|\boldsymbol{\psi}(x')|n+1) \cdot \left(n+1|\boldsymbol{\psi}^{\dagger}(x)|n\right) \tag{10b}$$

which act in the $n$-th subspace. By first applying Equation 6 and then Equation 8 we find

$$\begin{aligned} A_n \cdot \psi\left(x_1, x_2, \ldots, x_n\right) = {} & \delta\left(x_1 - x\right) \cdot \psi\left(x', x_2, \ldots, x_n\right) + \cdots \\ & + \varepsilon^{k-1} \cdot \delta\left(x_k - x\right) \cdot \psi\left(x', x_1, \ldots, x_{k-1}, x_{k+1}, \ldots, x_n\right) + \cdots \\ & + \varepsilon^{n-1} \cdot \delta\left(x_n - x\right) \cdot \psi\left(x', x_1, \ldots, x_{n-1}\right) , \end{aligned} \tag{11}$$

or, if we take into account the symmetry property of the wave function,

$$\begin{aligned} & \left(n|\boldsymbol{\psi}^{\dagger}(x) \cdot \boldsymbol{\psi}(x')|n\right) \cdot \psi\left(x_1, x_2, \ldots, x_n\right) \\ = {} & \delta\left(x_1 - x\right) \cdot \psi\left(x', x_2, \ldots, x_n\right) + \cdots + \delta\left(x_k - x\right) \\ & \cdot \psi\left(x_1, \ldots, x_{k-1}, x', x_{k+1}, \ldots, x_n\right) \\ & + \cdots + \delta\left(x_n - x\right) \cdot \psi\left(x_1, x_2, \ldots, x_{n-1}, x'\right) . \end{aligned} \tag{11a}$$

If one first applies Equation 8 and then Equation 6 and replaces $n$ by $n+1$, one finds:

$$\begin{aligned} B_n \cdot \psi\left(x_1, x_2, \ldots, x_n\right) = {} & \left(n|\boldsymbol{\psi}(x') \cdot \boldsymbol{\psi}^{\dagger}(x)|n\right) \cdot \psi\left(x_1, x_2, \ldots, x_n\right) \\ = {} & \delta\left(x' - x\right) \cdot \psi\left(x_1, x_2, \ldots, x_n\right) + \varepsilon \cdot \delta\left(x_1 - x\right) \cdot \psi\left(x', x_2, \ldots, x_n\right) + \cdots \\ & + \varepsilon^{k} \cdot \delta\left(x_k - x\right) \cdot \psi\left(x', x_1, \ldots, x_{k-1}, x_{k+1}, \ldots, x_n\right) + \cdots \\ & + \varepsilon^{n} \cdot \delta\left(x_n - x\right) \cdot \psi\left(x', x_1, \ldots, x_{n-1}\right) . \end{aligned} \tag{12}$$

Comparing Equation 11 and Equation 12 shows that

$$\begin{aligned} B_n \cdot \psi\left(x_1, x_2, \ldots, x_n\right) - \varepsilon \cdot A_n \cdot \psi\left(x_1, x_2, \ldots, x_n\right) = {} & \delta\left(x - x'\right) \\ & \cdot \psi\left(x_1, x_2, \ldots, x_n\right) . \end{aligned} \tag{13}$$

According to Equation 9a and Equation 9b this means that the commutation relation

$$\boldsymbol{\psi}(x') \cdot \boldsymbol{\psi}^{\dagger}(x) - \varepsilon \cdot \boldsymbol{\psi}^{\dagger}(x) \cdot \boldsymbol{\psi}(x') = \delta\left(x - x'\right) \tag{2a}$$

exists, where the identity matrix (with respect to $n$) must be added to the right.

Proving Equation 2b is even easier. According to Equation 6, the operator $\boldsymbol{\psi}(x)$ transforms the sequence of functions according to Equation 5 into

$$\left\{\begin{matrix} \psi(x) \\ \sqrt{2}\cdot\psi(x,x_1) \\ \sqrt{3}\cdot\psi(x,x_1,x_3) \\ \cdots\cdots \end{matrix}\right\},$$

i.e.

$$\boldsymbol{\psi}(x) = \left\{\begin{matrix} \text{const.} \\ \psi(x_1) \\ \psi(x_1,x_2) \\ \psi(x_1,x_2,x_3) \\ \cdots\cdots \end{matrix}\right\} = \left\{\begin{matrix} \psi(x) \\ \sqrt{2}\cdot\psi(x,x_1) \\ \sqrt{3}\cdot\psi(x,x_1,x_2) \\ \cdots\cdots \\ \cdots\cdots \end{matrix}\right\}. \tag{14}$$

If one applies the operator $\boldsymbol{\psi}(x')$ to Equation 14, one gets

$$\boldsymbol{\psi}(x')\cdot\boldsymbol{\psi}(x) = \left\{\begin{matrix} \text{const.} \\ \psi(x_1) \\ \psi(x_1,x_2) \\ \psi(x_1,x_2,x_3) \\ \cdots\cdots \end{matrix}\right\} = \left\{\begin{matrix} \sqrt{2\cdot 1}\cdot\psi(x,x') \\ \sqrt{3\cdot 2}\cdot\psi(x,x',x_1) \\ \sqrt{4\cdot 3}\cdot\psi(x,x',x_1,x_2) \\ \cdots\cdots\cdots\cdots \\ \cdots\cdots\cdots\cdots \end{matrix}\right\}. \tag{15a}$$

By exchanging $x$ with $x'$ one gets

$$\boldsymbol{\psi}(x)\cdot\boldsymbol{\psi}(x') = \left\{\begin{matrix} \text{const.} \\ \psi(x_1) \\ \psi(x_1,x_2) \\ \psi(x_1,x_2,x_3) \\ \cdots\cdots \end{matrix}\right\} = \left\{\begin{matrix} \sqrt{2\cdot 1}\cdot\psi(x',x) \\ \sqrt{3\cdot 2}\cdot\psi(x',x,x_1) \\ \sqrt{4\cdot 3}\cdot\psi(x',x,x_1,x_2) \\ \cdots\cdots\cdots\cdots \\ \cdots\cdots\cdots\cdots \end{matrix}\right\}. \tag{15b}$$

Now the expressions according to Equation 15a and Equation 15b are either equal ($\varepsilon = +1$, symmetric functions) or oppositely equal ($\varepsilon = -1$, antisymmetric functions), which proves Equation 2b.

With the help of the formulæ obtained, all operators of the second quantization can be constructed using the coordinate-space-method. Those of them that are not commutative with $\mathtt{m}$ act on sequences of functions of the kind according to Equation 5 and cannot be represented in a space of a certain number of dimensions. For the operators that can be commutated with $\mathtt{m}$, it is sufficient to consider the diagonal element of the matrix with respect to $n$, which can be viewed as an operator in the $n$-th subspace, i.e. in the

configuration space for a fixed number $n$ of particles. For example, the energy operator according to Equation 50 is commutative with respect to $\mathtt{m}$, and its construction in the configuration space leads back to the usual SCHRÖDINGER energy operator for $n$ particles. Here we want to look at a few more examples of the operators that can be commuted with respect to $\mathtt{m}$.

The operator $\boldsymbol{\psi}^{\dagger}(x) \cdot \boldsymbol{\psi}(x)$ of the particle density has the representation

$$\begin{aligned}&\left(n|\boldsymbol{\psi}^{\dagger}(x) \cdot \boldsymbol{\psi}(x)|n\right) \psi\left(x_1, x_2, \ldots, x_n\right) \\ &= \left\{\delta\left(x_1 - x\right) + \delta\left(x_2 - x\right) + \cdots + \delta\left(x_n - x\right)\right\} \cdot \psi\left(x_1, x_2, \ldots, x_n\right) .\end{aligned} \tag{16}$$

in the $n$-th subspace. This formula is a special case of Equation 11, which is obtained by setting $x' = x$ in Equation 11 and using the relation

$$\delta\left(x_k - x\right) \cdot f(x) = \delta\left(x_k - x\right) \cdot f(x_k)$$

valid for every continuous function $f(x)$.

If we multiply Equation 16 by the volume element $\mathrm{d}x$ and integrate over a subvolume $V$, we can conclude that the operator

$$\mathtt{m}_V = \int_V \boldsymbol{\psi}^{\dagger}(x) \cdot \boldsymbol{\psi}(x)\, \mathrm{d}x \tag{17}$$

in the $n$-th subspace has the following representation:

$$(n|\, \mathtt{m}_V\, |n) \cdot \psi\left(x_1, x_2, \ldots, x_n\right) = n'_V\left(x_1, x_2, \ldots, x_n\right) \cdot \psi\left(x_1, x_2, \ldots, x_n\right) . \tag{18}$$

The value of the function $n'_V\left(x_1, x_2, \ldots, x_n\right)$, which is multiplied in Equation 18, is equal to the number of arguments $x_1, x_2, \ldots, x_n$ that belong in the subvolume $V$. The operator $(n|\, \mathtt{m}_V\, |n)$ therefore has integer eigenvalues $n'_V = 0, 1, 2, \ldots, n$, as required.

As a further example, we consider the operator for the COULOMB potential

$$\mathsf{V}(\mathfrak{r}) = e_0^2 \cdot \int \frac{\boldsymbol{\psi}^{\dagger}(x) \cdot \boldsymbol{\psi}(x')}{|\mathfrak{r} - \mathfrak{r}'|}\, \mathrm{d}x' . \tag{19}$$

To form its matrix element $(n|\, \mathsf{V}(\mathfrak{r})|n)$, we replace $x$ in Equation 16 with $x'$, multiply by $\frac{e_0^2}{|\mathfrak{r}-\mathfrak{r}'|}$ and integrate over $x'$. We obtain

$$(n|\, \mathsf{V}(\mathfrak{r})|n) \cdot \psi\left(x_1, x_2, \ldots, x_n\right) = \sum_{k=1}^{n} \frac{e_0^2}{|\mathfrak{r} - \mathfrak{r}_k|} \cdot \psi\left(x_1, x_2, \ldots, x_n\right) . \tag{20}$$

The operator $\mathsf{V}(\mathfrak{r})$ therefore means a "multiplication by $\sum_{k=1}^{n} \frac{e_0^2}{|\mathfrak{r}-\mathfrak{r}_k|}$" in the $n$-th subspace.

## 2.1 Time dependence of the $\psi$ operators and the quantized wave equation

As is well known, the change in the state of a physical system over time is expressed either in the time dependence of the wave functions or in that of the operators. According to Dirac, [2], we refer to the representation of the operators that corresponds to the time-dependent wave functions as the Schrödinger and the one corresponding to the time-dependent matrices as the Heisenberg depiction.

Let $\psi$ be the wave function of the system and $S(t)$ be the unitary operator[7], which converts the initial value $\psi(\cdot, 0)$ of the wave function into its value $\psi(\cdot, t)$ at time $t$. (The variables of the system are indicated here with a dot.) We have

$$\psi(\cdot, t) = S(t) \cdot \psi(\cdot, 0)\,. \tag{21}$$

If one differentiates this equation according to time and replace $\psi(\cdot, 0)$ by

$$\psi(\cdot, 0) = S^{\dagger}(t) \cdot \psi(\cdot, t)\,, \tag{21a}$$

one gets

$$\frac{\partial\psi}{\partial t} = \dot{S}(t) \cdot \psi(\cdot, 0) = \dot{S}(t) S^{\dagger}(t) \cdot \psi(\cdot, t)\,. \tag{22}$$

We denote the Hermitian operator $\mathtt{i}\,\dot{S} S^{\dagger}$ as

$$\mathtt{i}\,\dot{S}(t) S^{\dagger}(t) = -\,\mathtt{i}\,S(t)\dot{S}^{\dagger}(t) = \frac{1}{\hbar} \cdot \mathscr{H}\,, \tag{23}$$

because $S S^{\dagger} = 1$. $\mathscr{H}$ is then the Hamilton operator of the system. If we denote by $L$ an operator in the Schrödinger representation, and by $L'(t)$ the same operator in the Heisenberg representation, we have

$$L'(t) = S^{\dagger}(t) L S(t)\,. \tag{24}$$

From Equation 24 and Equation 21 there results

$$L'(t)\psi(\cdot, 0) = S^{\dagger}(t) L \psi(\cdot, t)\,. \tag{25}$$

The time derivative of this expression is equal to

$$\frac{\mathrm{d}L'(t)}{\mathrm{d}t}\psi(\cdot, 0) = \frac{\mathrm{d}}{\mathrm{d}t}\left(S^{\dagger}(t) L \psi(\cdot, t)\right)\,. \tag{26}$$

On the left is the operator $\frac{\mathrm{d}L'(t)}{\mathrm{d}t}$ in the Heisenberg representation. If we denote the same operator in the Schrödinger representation with $\frac{\mathrm{d}L(t)}{\mathrm{d}t}$, we have, analogous to Equation 24 and Equation 25

$$\frac{\mathrm{d}L'(t)}{\mathrm{d}t} = S^{\dagger}(t) \cdot \frac{\mathrm{d}L}{\mathrm{d}t} S(t) \tag{27}$$

[7] see `https://en.wikipedia.org/wiki/Unitary_operator`

and

$$\frac{\mathrm{d}L'(t)}{\mathrm{d}t}\psi(\cdot,0) = S^{\dagger}(t)\cdot\frac{\mathrm{d}L}{\mathrm{d}t}\psi(\cdot,t)\,. \tag{28}$$

Comparing Equation 26 and Equation 28 yields

$$\frac{\mathrm{d}L}{\mathrm{d}t}\psi(\cdot,t) = S(t)\cdot\frac{\mathrm{d}}{\mathrm{d}t}\left(S^{\dagger}(t)L\psi(\cdot,t)\right)\,, \tag{29}$$

or, if one performs the differentiations,

$$\frac{\mathrm{d}L}{\mathrm{d}t}\psi(\cdot,t) = S(t)\dot{S}^{\dagger}(t)L\psi(\cdot,t) + \frac{\mathrm{d}}{\mathrm{d}t}\left(L\psi(\cdot,t)\right)\,. \tag{30}$$

Note that according to Equation 21 (or according to Equation 21a) the operator $S(t)$ (or $S^{\dagger}(t)$) causes the temporal continuation of the wave function around time $t$ in the positive (or in the negative) sense, the content of Equation 29 can be formulated as follows.

In the Schrödinger representation one gets the result of applying the operator $\frac{\mathrm{d}L}{\mathrm{d}t}$ to the wave functions $\psi(\cdot,t)$ if one carries out the following operations:

1. Application of the operator $L$.
2. Time continuation in negative time direction around time $t$.
3. Differentiate according to time.
4. Time continuation in positive time direction around time $t$.

This formulation has the advantage that the Hamilton operator is not used explicitly.

This rule can now be applied to the determination of the operator $\frac{\partial\boldsymbol{\psi}}{\partial t}$, which appears in the quantized wave equation. The operator $L$ in this case is the quantized wave function $\boldsymbol{\psi}(x,t)$ and $\psi(\cdot,t)$ is the function sequence according to Equation 5. We limit ourselves to the case where the number of particles does not change over time and thereby exclude the consideration of photons. To obtain more descriptive formulæ, we consider the quantized Schrödinger equation

$$\left[H^0(x) + \mathsf{V}(x)\right]\boldsymbol{\psi}(x) = \mathtt{i}\,\hbar\cdot\frac{\partial\boldsymbol{\psi}}{\partial t}\,, \tag{31}$$

where $H^0(x)$ denotes the ordinary Schrödinger operator of the one-body problem:

$$H^0(x) = -\frac{\hbar^2}{2m}\cdot\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right) + U(x,y,z) \tag{32}$$

and $\mathsf{V}(x) = \mathsf{V}(\mathfrak{r})$ is the operator for the Coulomb potential defined by Equation 19.

In our case, the operator $S(t)$ in the configuration space simply causes the temporal continuation of the individual wave functions $\psi(x_1, x_2, \ldots, x_n; t)$ of the sequence according to Equation 5

$$S(t)\left\{\begin{array}{c} \text{const.} \\ \psi(x_1;0) \\ \psi(x_1,x_2;0) \\ \psi(x_1,x_2,x_3;0) \\ \cdots\cdots \end{array}\right\} = \left\{\begin{array}{c} \text{const.} \\ \psi(x_1;t) \\ \psi(x_1,x_2;t) \\ \psi(x_1,x_2,x_3;t) \\ \cdots\cdots \end{array}\right\}. \tag{33}$$

So the operator $S(t)$ has the diagonal form

$$S(t) = \left\{\begin{array}{ccccc} S_0 & 0 & 0 & 0 & \vdots \\ 0 & S_1 & 0 & 0 & \vdots \\ 0 & 0 & S_2 & 0 & \vdots \\ 0 & 0 & 0 & S_3 & \vdots \\ \cdots & \cdots & \cdots & \cdots & \end{array}\right\}, \tag{34}$$

where $S_n = S_n(t)$ is an operator that continues the wave function in time in the $n$-th subspace:

$$S_n(t) \cdot \psi(x_1, x_2, \ldots, x_n; 0) = \psi(x_1, x_2, \ldots, x_n; t) \tag{35}$$

We also have according to Equation 23

$$-\mathtt{i}\,\hbar \cdot S_n(t)\dot{S}_n^\dagger(t) = \mathscr{H}(x_1, x_2, \ldots, x_n) \tag{36}$$

where $\mathscr{H}(x_1, x_2, \ldots, x_n)$ denotes the Hamilton operator in the $n$-th subspace. The operator $-\mathtt{i}\,\hbar \cdot S\dot{S}^\dagger$ is also a diagonal operator with Equation 36 as diagonal elements.

We now form the operator $\dot{\boldsymbol{\psi}}(x;t) = \frac{\partial \psi}{\partial t}$. We have according to Equation 29 or Equation 30

$$\begin{aligned} \dot{\boldsymbol{\psi}}(x;t)&\left\{\begin{array}{c} \text{const.} \\ \psi(x_1;t) \\ \psi(x_1,x_2;t) \\ \psi(x_1,x_2,x_3;t) \\ \cdots\cdots\cdots \end{array}\right\} \\ &= S(t)\dot{S}^\dagger(t)\left\{\begin{array}{c} \psi(x;t) \\ \sqrt{2}\cdot\psi(x,x_1;t) \\ \sqrt{3}\cdot\psi(x,x_1,x_2;t) \\ \cdots\cdots\cdots\cdots \end{array}\right\} + \left\{\begin{array}{c} \dot{\psi}(x;t) \\ \sqrt{2}\cdot\dot{\psi}(x,x_1;t) \\ \sqrt{3}\cdot\dot{\psi}(x,x_1,x_2;t) \\ \cdots\cdots\cdots\cdots \end{array}\right\}, \end{aligned} \tag{37}$$

and if we consider Equation 36

$$
\begin{aligned}
&\mathtt{i}\,\hbar\cdot\dot{\boldsymbol{\psi}}(x;t)\left\{\begin{matrix}\text{const.}\\ \psi\,(x_1;t)\\ \psi\,(x_1,x_2;t)\\ \cdots\cdots\end{matrix}\right\}\\
&=\left\{\begin{matrix}0\\ -\sqrt{2}\cdot\mathscr{H}(x_1)\psi\,(x,x_1;t)\\ -\sqrt{3}\cdot\mathscr{H}(x_1,x_2)\psi\,(x,x_1,x_2;t)\\ \cdots\cdots\cdots\cdots\cdots\cdots\end{matrix}\right\}+\mathtt{i}\,\hbar\left\{\begin{matrix}\dot{\psi}(x;t)\\ \sqrt{2}\cdot\dot{\psi}(x,x_1;t)\\ \sqrt{3}\cdot\dot{\psi}(x,x_1,x_2;t)\\ \cdots\cdots\cdots\cdots\end{matrix}\right\}.
\end{aligned}
\tag{38}
$$

For the operator on the left side of the quantized wave equation according to Equation 31, we get, if we take Equation 20 into account,

$$
\begin{aligned}
&\left[H^0(x)\cdot\boldsymbol{\psi}+\mathsf{V}(x)\cdot\boldsymbol{\psi}\right]\left\{\begin{matrix}\text{const.}\\ \psi(x_1;t)\\ \psi(x_1,x_2;t)\\ \cdots\cdots\end{matrix}\right\}\\
&=\left[H^0(x)+\mathsf{V}(x)\right]\left\{\begin{matrix}\psi(x;t)\\ \sqrt{2}\cdot\psi(x,x_1;t)\\ \sqrt{3}\cdot\psi(x,x_1,x_2;t)\\ \cdots\cdots\cdots\cdots\end{matrix}\right\}\\
&=\left\{\begin{matrix}H^0(x)\psi(x;t)\\ \sqrt{2}\cdot\left[H^0(x)+\frac{e_0^2}{|\mathfrak{r}-\mathfrak{r}_1|}\right]\cdot\psi(x,x_1;t)\\ \sqrt{3}\cdot\left[H^0(x)+\frac{e_0^2}{|\mathfrak{r}-\mathfrak{r}_1|}+\frac{e_0^2}{|\mathfrak{r}-\mathfrak{r}_2|}\right]\cdot\psi(x,x_1,x_2;t)\\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\end{matrix}\right\}.
\end{aligned}
\tag{39}
$$

By equating Equation 38 and Equation 39 we get (after dividing by $\sqrt{2}$, $\sqrt{3}$, etc.) a

chain of equations

$$H^0(x) \cdot \psi(x;t) = \mathtt{i}\,\hbar \cdot \frac{\partial \psi(x;t)}{\partial t}\,, \tag{40$_1$}$$

$$\left[H^0(x) + \frac{e_0^2}{|\mathfrak{r} - \mathfrak{r}_1|} + \mathscr{H}(x_1)\right] \cdot \psi(x, x_1; t) = \mathtt{i}\,\hbar \cdot \frac{\partial}{\partial t}\psi(x, x_1; t)\,, \tag{40$_2$}$$

$$\left[H^0(x) + \frac{e_0^2}{|\mathfrak{r} - \mathfrak{r}_1|} + \frac{e_0^2}{|\mathfrak{r} - \mathfrak{r}_2|} + \mathscr{H}(x_1, x_2)\right]$$
$$\cdot\, \psi(x, x_1, x_2; t) = \mathtt{i}\,\hbar \cdot \frac{\partial}{\partial t}\psi(x, x_1, x_2; t)\,, \tag{40$_3$}$$

$$\left[H^0(x) + \sum_{k=1}^{n} \frac{e_0^2}{|\mathfrak{r} - \mathfrak{r}_k|} + \mathscr{H}(x_1, x_2, \ldots, x_n)\right]$$
$$\cdot\, \psi(x, x_1, x_2, \ldots, x_n; t) = \mathtt{i}\,\hbar \cdot \frac{\partial}{\partial t}\psi(x, x_1, x_2, \ldots, x_n; t)\,. \tag{40$_{\mathrm{n+1}}$}$$

From Equation 40 one can see that

$$\mathscr{H}(x) = H^0(x)\,;$$

is satisfied; Equation $40_2$ then returns

$$\mathscr{H}\,(x, x_1) = H^0(x) + H^0\,(x_1) + \frac{e_0^2}{|\mathfrak{r} - \mathfrak{r}_1|} \text{ etc.}$$

In general, the $(n + 1)$-th equation provides a recursion relation between the Schrödinger operator for $n$ and for $(n + 1)$ particles, namely

$$\mathscr{H}\,(x, x_1, x_2, \ldots, x_n) = H^0\,(x) + \sum_{k=1}^{n} \frac{e_0^2}{|\mathfrak{r} - \mathfrak{r}_k|} + \mathscr{H}\,(x_1, x_2, \ldots, x_n)\;. \tag{41}$$

If one now expresses $\mathscr{H}\,(x_1, x_2, \ldots, x_n)$ directly in terms of $H^0$, one gets for the Hamilton operator of the $n$-body problem the common Schrödinger expression

$$\mathscr{H}\,(x_1, x_2, \ldots, x_n) = \sum_{k=1}^{n} H^0\,(x_k) + \sum_{k>l=1}^{n} \frac{e_0^2}{|\mathfrak{r}_k - \mathfrak{r}_l|}\,. \tag{42}$$

The quantized wave equation, Equation 31, therefore breaks down in the configuration space into a sequence of ordinary Schrödinger equations according to

$$\mathscr{H}\,(x_1, x_2, \ldots, x_n) \cdot \psi\,(x_1, x_2, \ldots, x_n; t) = \mathtt{i}\,\hbar \cdot \frac{\partial \psi}{\partial t}\,. \tag{43}$$

This example shows that computing with quantized wave functions allows an immediate transition to the usual configuration space at every stage.

## 2.2 Derivation of Hartree's equations using the method of second quantization

As a simple application of the results obtained, we want to derive the HARTREE equations, [4], supplemented by taking the exchange into account.

As is well known, the equations for the eigenfunctions of the energy operator (as well as the HARTREE equations) can be derived from the variational principle

$$\delta W = 0\,, \tag{44}$$

where $W$ denotes the energy of the atom in the considered stationary state. It is therefore sufficient to find the expression for the energy. But now $W$ is equal to the diagonal element

$$W = (Wn|\,\mathbb{H}\,|Wn) \tag{45}$$

of the matrix for the quantized energy operator $\mathbb{H}$ (see Equation 50 of the first part):

$$\begin{aligned}\mathbb{H} = &\int \boldsymbol{\psi}^\dagger(x)\cdot H(x)\cdot \boldsymbol{\psi}(x)\,\mathrm{d}x\\ &+ \frac{e_0^2}{2}\cdot \iint \frac{\boldsymbol{\psi}^\dagger(x)\cdot\boldsymbol{\psi}^\dagger(x')\cdot\boldsymbol{\psi}(x')\cdot\boldsymbol{\psi}(x)}{|\mathfrak{r}-\mathfrak{r}'|}\,\mathrm{d}x\,\mathrm{d}x'\,.\end{aligned} \tag{46}$$

To determine $W$, we need to calculate the matrix elements of the operators under the integral sign.

We have

$$\begin{gathered}\left(Wn|\boldsymbol{\psi}^\dagger(x)\cdot H(x)\cdot\boldsymbol{\psi}(x)|Wn\right) = H(x')\cdot\left(Wn|\boldsymbol{\psi}^\dagger(x)\cdot\boldsymbol{\psi}(x')|Wn\right)\\ \text{for } x' = x\,.\end{gathered} \tag{47}$$

To calculate the matrix element of the operator in the first integral, it is sufficient to determine the quantity

$$\varrho(x,x') = \left(Wn|\boldsymbol{\psi}^\dagger(x)\cdot\boldsymbol{\psi}(x')|Wn\right)\,. \tag{48}$$

We have already found the expression for the operator $\boldsymbol{\psi}^\dagger(x)\cdot\boldsymbol{\psi}(x')$ in the $n$-th subspace (see Equation 11a); With the help of the eigenfunction $\psi_W(x_1,x_2,\ldots,x_n)$ of the energy operator in the $n$-th subspace, which belongs to the eigenvalue $W$, we get from this if we take into account the symmetry property of the wave function,

$$\varrho(x,x') = n\cdot\int\cdots\int \overline{\psi}_w\cdot(x,x_2,\ldots,x_n)\cdot\psi_w\,(x',x_2,\ldots,x_n)\,\mathrm{d}x_2\cdots\mathrm{d}x_n\,. \tag{49}$$

To derive the HARTREE equations, we must replace the wave functions in this exact expression with an approximate expression in determinant form according to

$$\psi_w(x_1, x_2, \ldots, x_n) = \frac{1}{\sqrt{n!}} \cdot \|\varphi_i(x_k)\| \quad (i, k = 1, 2, 3, \ldots, n) \tag{50}$$

where the $\varphi_i(x)$ are assumed to be orthogonal and normalized:

$$\int \overline{\varphi}_i(x) \cdot \varphi_k(x)\, \mathrm{d}x = \delta_{ik}\,. \tag{51}$$

We then get

$$\varrho(x, x') = \sum_{i=1}^{n} \overline{\varphi}_i(x) \cdot \varphi_i(x')\,, \tag{49a}$$

and consequently, according to Equation 47 and Equation 48,

$$\left(Wn|\boldsymbol{\psi}^\dagger(x) \cdot H(x) \cdot \boldsymbol{\psi}(x)|Wn\right) = \sum_{i=1}^{n} \overline{\varphi}_i(x) \cdot H(x) \cdot \varphi_i(x)\,. \tag{52}$$

We now calculate the matrix element of the operator in the double integral in Equation 46. Using Equation 14, Equation 16 and Equation 8 one easily finds that this operator has the following meaning in the $n$-th subspace:

$$\begin{aligned} &\left(n|\boldsymbol{\psi}^\dagger(x) \cdot \boldsymbol{\psi}^\dagger(x') \cdot \boldsymbol{\psi}(x') \cdot \boldsymbol{\psi}(x)|n\right) \cdot \psi(x_1, x_2, \ldots, x_n) \\ = &\sum_{\substack{k,l=1 \\ (k \neq l)}}^{n} \delta(x_k - x) \cdot \delta(x_l - x') \cdot \psi(x_1, x_2, \ldots, x_n)\,. \end{aligned} \tag{53}$$

Consequently, its matrix element is equal to

$$\begin{aligned} &\left(Wn|\boldsymbol{\psi}^\dagger(x) \cdot \boldsymbol{\psi}^\dagger(x') \cdot \boldsymbol{\psi}(x') \cdot \boldsymbol{\psi}(x)|Wn\right) \\ = \; &n \cdot (n-1) \cdot \int \cdots \int \left|\psi_W(x, x', x_3, \ldots, x_n)\right|^2 \mathrm{d}x_3 \cdots \mathrm{d}x_n\,. \end{aligned} \tag{54}$$

After inserting the determinant expression according to Equation 50 for $\psi_W$, the approximate formula is obtained from Equation 54 (cf. [3])

$$\left(Wn|\boldsymbol{\psi}^\dagger(x) \cdot \boldsymbol{\psi}^\dagger(x') \cdot \boldsymbol{\psi}(x') \cdot \boldsymbol{\psi}(x)|Wn\right) = \varrho(x, x) \cdot \varrho(x', x') - |\varrho(x, x')|^2\,. \tag{55}$$

If one now introduces Equation 52 and Equation 55 into Equation 46, one gets for the matrix element of $\mathbb{H}$, i.e. for the energy $W$ the expression

$$\begin{aligned} W = &\int \sum_{i=1}^{n} \overline{\varphi}_i(x) \cdot H(x) \cdot \varphi_i(x)\, \mathrm{d}x \\ &+ \frac{e_0^2}{2} \cdot \iint \frac{\varrho(x, x) \cdot \varrho(x', x') - |\varrho(x, x')|^2}{|\mathfrak{r} - \mathfrak{r}'|}\, \mathrm{d}x\, \mathrm{d}x'\,. \end{aligned} \tag{56}$$

This expression only differs from the one given in our cited work, see [4] (formula (93)), in that here we consider the spin coordinate included in the variable $x$ and are therefore entitled to operate with purely antisymmetric wave functions.

Leningrad, Physical-Technical Institute.

# References


[1] P. A. M. Dirac. The quantum theory of the emission and absorption of radiation. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 114(767):243–265, 1927. On the introduction of the second quantization (Bose Statistics without interaction).

[2] P. A. M. Dirac. *The principles of Quantum Mechanics*. Oxford University Press, 1st edition, 1930. see §38.

[3] P. A. M. Dirac. Note on the Interpretation of the Density Matrix in the Many-Electron Problem. *Mathematical Proceedings of the Cambridge Philosophical Society*, 27(2):240–243, 1931.

[4] V. Fock. Näherungsmethode zur Lösung des quantenmechanischen Mehrkörperproblems. *Zeitschrift für Physik*, 61(1-2):126–148, 1930.

[5] P. Jordan. Zur Quantenmechanik der Gasentartung. *Zeitschrift für Physik*, 44(6-7):473–480, 1927. On Fermi Statistics.

[6] P. Jordan. Über Wellen und Korpuskeln in der Quantenmechanik. *Zeitschrift für Physik*, 45(11-12):766–775, 1927. On the Bose Statistics with interaction.

[7] P. Jordan. Zur Methode der zweiten Quantelung. *Zeitschrift für Physik*, 75(9-10):648–653, 1932.

[8] P. Jordan and O. Klein. Zum Mehrkörperproblem der Quantentheorie. *Zeitschrift für Physik*, 45(11-12):751–765, 1927. On the Bose Statistics with interaction.

[9] P. Jordan and E. Wigner. Über das Paulische Äquivalenzverbot. *Zeitschrift für Physik*, 47(9-10):631–651, 1928. On Fermi Statistics.

[10] L. Landau and R. Peierls. Quantenelektrodynamik im Konfigurationsraum. *Zeitschrift für Physik*, 62(3-4):188–200, 1930.